REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
16-12-02

2. REPORT TYPE
Technical Paper

3. DATES COVERED *(From - To)*

4. TITLE AND SUBTITLE

Three-Dimensional Simulations of a Gas/Gas, Hydrogen/Oxygen Engine

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

Mark R. Archambault[1]
Oshin Peroomian[2]

5d. PROJECT NUMBER
3058

5e. TASK NUMBER
RF9A

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

[1]Air Force Research Laboratory (AFMC)
AFRL/PRSA
10 E. Saturn Blvd.
Edwards AFB, CA 93524-7680

[2]Metacomp Technologies, Inc.
Agoura Hills, CA 91301

8. PERFORMING ORGANIZATION REPORT NUMBER

AFRL-PR-ED-TP-2002-309

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory (AFMC)
AFRL/PRS
5 Pollux Drive
Edwards AFB CA 93524-7048

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S NUMBER(S)
AFRL-PR-ED-TP-2002-309

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
					Leilani Richardson
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**	A	11	**19b. TELEPHONE NUMBER** *(include area code)*
Unclassified	**Unclassified**	**Unclassified**			(661) 275-5015

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. 239.18

AIAA-2003-0314

THREE-DIMENSIONAL SIMULATIONS OF A GAS/GAS, HYDROGEN/OXYGEN ENGINE

Mark R. Archambault*

Air Force Research Laboratory
Propulsion Directorate
Space and Missile Propulsion Division
Edwards AFB, CA 93524

Oshin Peroomian†

Metacomp Technologies, Inc.
Agoura Hills, CA 91301

20080814 237

Abstract

As part of an ongoing program to develop a computational methodology to obtain high-fidelity rocket engine flow solutions, three-dimensional, time-accurate computations were performed on a single-element, shear-coaxial, gas/gas, H_2/O_2 rocket engine. The purpose of the present work is to determine what level of model fidelity is required to capture the essential physical behavior of the flow. The simulations discussed here are of the highest fidelity thus far reported and represent the leading edge of numerical modeling capability for this class of problems. Results are compared with previous two-dimensional calculations, showing that the time-accurate simulations better represent the experimental data in most cases, and that the three-dimensional calculations do as well as or slightly better at predicting the data. Additionally, while no three-dimensional patterns (such as a helical structure) are present in the shear layer, the three-dimensional calculation does predict other differences from the two-dimensional calculation such as a shift in the position of the upstream recirculation zone. Continued learning and understanding are required to further push the envelope of high fidelity simulations while at the same time making them faster, more efficient, and more robust than they are today.

Introduction

Staged combustion cycle engines, such as the H_2/O_2 Integrated Powerhead Demo or a staged combustion hydrocarbon boost engine, have become a focus of research within the rocket propulsion community. In support of this research, ongoing computational and experimental efforts have advanced the development of a design methodology for gas/gas injectors. The goal is to use experimental measurements to anchor state-of-the-art codes which can then be used to investigate a series of injector configurations. This provides a more efficient design process, resulting in significant savings in full-scale development time and costs.

This paper focuses on continuing efforts to develop a computational methodology to efficiently, accurately, and robustly obtain high-fidelity solutions of combusting rocket engines so as to gain a knowledge and understanding of their features. Three-dimensional simulations of a combusting, single-element, shear-coaxial, H_2/O_2 engine were performed to investigate the degree of modeling fidelity required to reproduce the essential physical behavior of the flow. Experimental data are shown for comparison to help illustrate the conclusions.

This class of problems has been previously investigated both experimentally[1,2] and computationally.[2,3,4,5,6] The experiments produced data

*Aerospace Engineer
†Computer Scientist

on hydrogen and oxygen mole fractions, mean and RMS velocities, and OH-radical concentration. This problem has since been used as a benchmark for assessing CFD capabilities for designing gas/gas injectors within a rocket combustor environment. Recent computational investigations[5] showed that solutions could be achieved on finer grids than previously reported[2,4] using a second-order, implicit, upwind, preconditioning scheme. These solutions compare well with experiment and reveal additional structure near the injectors. It was also shown in Reference 5 that a time-averaged transient solution produces a different result than does a steady solution due to the inherently unsteady nature of coaxial shear flows. It has also been previously shown[6] that modeling features that are present in an experimental setup, but not likely to be present in actual flight hardware, can have a significant impact upon the solution results. For example, it was shown that including the nitrogen curtain purge that cooled the diagnostic windows in the experiment significantly altered the predicted hydrogen mole fraction profiles.

In the present study, the authors examine what features of the flow are predicted from a fully three-dimensional geometry. Previously, the engine was modeled using an axisymmetric geometry. This was a departure from the actual geometry in the sense that the actual engine has a square cross-section and the circular diagnostic windows are only located on the top and bottom of the chamber. By introducing three-dimensionality into the simulation, one can examine the effects of the actual geometry and determine if any three-dimensional flow features are present, such as a helical pattern, within the shear layer. It will also be possible to make an assessment as to what level of fidelity is necessary to adequately model this class of problems.

Computational Model

Results were obtained from the CFD++ flow solver from Metacomp Technologies, Inc.[7,8] The code has the capability to solve the Reynolds-Averaged Navier-Stokes (RANS) equations, the Large Eddy Simulation (LES) equations, or a RANS/LES hybrid set of equations on 3-D structured and unstructured grids. It is a compressible/incompressible flow code with high- and low-speed capability and has both finite-rate and frozen chemistry options. Low-speed flows are solved using a preconditioning algorithm. Explicit (Runge-Kutta) and implicit schemes are available for both steady and unsteady flows.

Schematics of the computational domain are shown in Figure 1. Hydrogen gas flows through an annulus surrounding a central core of gaseous oxygen. The gases enter the combustion chamber where they mix in a shear layer and react. The experimental hardware has a converging section at the end of the chamber which terminates at the throat where the gas is expelled to the atmosphere. In the computational setup, however, this section has been omitted to be consistent with previous calculations.[5,6]

Oxygen was injected into the chamber at a mass flow rate of 0.042 kg/s (0.1 lbm/sec) with an O/F ratio of 4. The chamber pressure was specified at 1.29 MPa and the inlet temperature at 297K. The injectors were modeled sufficiently upstream so that a fully-developed turbulent profile had formed by the time the gas enters the chamber. Standard subsonic boundary conditions were imposed at the outflow boundary, as well as no-slip conditions at solid surfaces.

Thirty-two processors of an SGI Origin 3800 computer ran the simulations at the Edwards Distributed Computing Center. CFD++ was set up to run the 3-D, compressible, real gas equations discretized with a second-order, upwind finite-volume scheme on a grid consisting of approximately 1.3 million cells. Stretching the grid resolved the region near the injectors and provided an adequate number of grid cells within the boundary layer inside the injectors. The time-accurate calculations were carried out using an implicit, preconditioned, dual time stepping algorithm. Combustion was handled using the Anderson 9-species, 19-reaction chemistry mechanism[9] solved with a finite-rate kinetics scheme and a constant-pressure combustion model. Turbulence was handled using a linear, realizable k-epsilon model.[10] The steady solution was initialized from a quiescent flow and ran for 3000 iterations at a nominal CFL number of 12. The transient calculation was initialized with the steady solution and ran time steps of 5 microseconds for 4500 iterations. After 1500 time steps, it was determined that the initial steady solution had moved out of the domain, and another 3000 time steps were performed where solution files were stored after ever 100 time steps. For each time step, 6 sub-iterations were performed, with the residual dropping approximately one order of magnitude by the end of those 6 sub-iterations.

Results

The results presented below represent the authors' first success at three-dimensional calculations on this class of problems and represent the greatest degree of fidelity of this class of problems reported to date. There is an ongoing learning process to determine the best and most efficient way to perform these types of calculations to make them faster and better than they currently are. Changes to the problem setup, such as additional grid refinement, the implementation of alternative turbulence models, and creative uses of symmetry have yet to be investigated. While the authors do not portray these results as the final word on this problem, they are obtained from the most rigorous calculations known to have been completed.

Figure 2 shows contour plots of OH concentration, a good indicator as to the location of the flame front. Each plot depicts a different level of fidelity. It is easy to see the similarities between the 3-D steady (Figure 2a) and 2-D time-averaged (Figure 2d) plots.[††] Based on these plots, one may argue that it seems that little is gained from increasing the degree of model fidelity from 2-D time-averaged to 3-D steady. However, it is important to remember that this is an inherently unsteady flow, and any steady solution will not be able to capture all of the flow dynamics, such as the flapping of the flame, movement of a recirculation zone, or any helical structures that might be present. Figure 2b illustrates this point by showing the asymmetric flapping of the flame. A comparison of Figures 2a and 2b show that the actual flame is thicker than the steady solution predicts, and the steady solution is not able to capture the motion of the flame. This is also seen from the 3-D time-averaged solution shown in Figure 2c. The steady and time-dependent solutions are significantly different.

One can also see differences among the various levels of fidelity in the species and velocity profiles. Figure 3 shows the hydrogen mole fraction profile at five inches downstream of the injector, corresponding to the axial location of the nitrogen curtain purge. Comparing the two-dimensional and three-dimensional results, the three-dimensional results seem to best represent the data. One must be mindful, however, to recognize that error bars are not present on the experimental data. The exact experimental uncertainties were not available at the time of writing, however, the species data were collected by Raman spectroscopy, which typically has an uncertainly of 30%. Using this value of uncertainty, it still appears that the three-dimensional results best capture the experimental results.

Another interesting point in Figure 3 comes from a comparison of the two-dimensional time-averaged curves with and without the nitrogen purge. Note that when the nitrogen purge is not present, the hydrogen has diffused further from the shear layer, resulting in a broader profile. When the nitrogen purge is active, the hydrogen does not demonstrate as much radial diffusion, and better represents the data. This is reasonable since the nitrogen purge was present in the experiment. This result has been previously reported[6] and strongly suggests that modeling the nitrogen purge is necessary when trying to reproduce data collected from this experiment. In the three-dimensional calculations, the nitrogen purge was also present. Considering that the time required to obtain the time-accurate three-dimensional solutions was several weeks, a simulation where the nitrogen purge was not present was not conducted. However, it is fair to extrapolate from the two-dimensional comparison that had the nitrogen purge been omitted in the three-dimensional calculation, it would have resulted in a broader hydrogen profile. The presence of the nitrogen has the effect of compacting or "hemming in" the hydrogen, not allowing it to diffuse outward as readily as when the nitrogen is absent. This stresses the need model all experimental features to ensure the most accurate representation of the experiment.

Figure 4 presents the oxygen mole fraction profile at five inches downstream from the injector. Although the profiles from the varying degrees of fidelity are very similar, showing little change from one case to the next, there are a few points to be made. First, there is clear disagreement between the calculation and experiment in the vicinity of $r/R_0=0$. However, examination of the experimental profile in this region suggests that the data may be faulty in some manner. The profile is not smooth, as one might expect, and there is no evidence that other species have diffused to the centerline of the flow. OH and O_2 contours from all the simulations suggest that the oxygen core continues for quite some distance downstream of the five-inch location. Thus, comparison of the numerical and experimental oxygen profiles near the centerline should be avoided.

Each level of fidelity seems to accurately predict the data within the shear layer between $r/R_0 = 0.5$ and 1.3, however further from the centerline, the time-averaged three-dimensional results diverge from the data. This could be caused by a couple different reasons. First, the grid in the vicinity of the shear layer may need some refinement. Currently, the grid near the shear layer is very dense near the injector lip, but gradually spreads out further downstream. Another cause could be the data itself. Because this is an unsteady flow, the flame flaps around, and there is no guarantee that when the data was being collected the shear layer remained in the probe volume. Because the data represents an average over the collection time, a flapping shear layer may manifest an over-prediction in the oxygen diffusion rate.

Finally, it should be noted that the curve that least represents the data is the one generated from the two-dimensional time-accurate calculation where the nitrogen purge is absent. This again suggests the need to model such experimental features. However, all the curves are quantitatively similar, and may fall within the experimental uncertainties.

[††] Previous two-dimensional calculations were run with a shorter chamber length. Considering the flow structure present at the end of the longer chamber in the three-dimensional calculations, the authors would like to reexamine the two-dimensional cases with the longer chamber. Future calculations will include the nozzle and throat geometry.

Figures 5 and 6 show profiles of the mean axial and RMS velocities, respectively. The greatest differences among the levels of fidelity appear in the mean velocity profile. Note that the two-dimensional simulations continue to show the peaks in the hydrogen gas, due to the greater injection velocity of the hydrogen. However, the three-dimensional solutions and the experimental results show that by the time the flow reaches five inches from the injectors the gas momentum has sufficiently diffused to eliminate those peaks. While this may be a function of the turbulence model, it may also be an indication that the three-dimensional nature of the chamber (i.e. the square geometry as opposed to an axisymmetric geometry) could be impacting on the velocity. This is important since velocity difference impacts upon the strength of the shear layer, and thus on mixing and combustion efficiency. The RMS profiles in Figure 6 are strongly dependent upon the turbulence model, however it would appear from the figure that the level of fidelity has little impact. Each of the curves seem to do about as well at predicting the experiment, though all tend to slightly under-predict the turbulence level near the centerline.

Another interesting feature is the pattern of nitrogen concentration (from the purge) throughout the chamber. Nitrogen contours are plotted in Figure 7, with the 2-D case on top, and the 3-D case on the bottom. The differences in the contours result from the slight forward movement of the upstream recirculation zone in the 3-D case. One can see from the streamtraces that are overlaid on the plot that in the 3-D case nitrogen is getting pulled into the recirculation zone, causing it to flow upstream and collect in the corners of the chamber. It can also be seen that nitrogen tends to diffuse more towards the centerline in the 3-D case than in the 2-D case. The reasons for these differences are most likely due to the differences in the chamber geometry. In the 2-D simulations, the chamber (including the nitrogen windows) were modeled axisymmetrically. Because the mass flow rate of nitrogen was held the same in both the 2-D and 3-D simulations, the injection velocity in the 2-D case was lower due to the greater injection area. These differences are important for the experimenter who might be relying on CFD predictions to develop an experiment. These results indicate that the nitrogen being used to cool optical access may not be flowing in the chamber as intended, which could result in biased experimental results at best, and damaged equipment at worst.

Finally, analysis of the data files from the time-accurate simulations showed no obvious three-dimensional flow patterns in the shear layer, such as a helical structure. Figure 8 shows contours of OH concentration taken from transverse slices in the chamber. These slices show a narrow ring of flame that does not significantly change in time, thought it does thicken as it moves downstream. If any sort of helical structure existed in the flow, one would expect to see variations of OH concentration in the azimuthal direction in time, yet none exist. The slight variations seen in the figure can be attributed to the presence of the nitrogen purge located on the top and bottom of chamber and the nitrogen being drawn back into the recirculation zone as previously discussed. Streamtrace analyses through the volume data also show no indication of induced swirl or helical structures. This is significant because it may mean that it is possible to do less-than-full three-dimensional simulations, but still capture many of the three-dimensional effects already discussed. Thus it might be possible to model the chamber with planar or wedge symmetry. Additional study on this is necessary.

It is important to keep in mind that the three-dimensional results presented in this work are preliminary and that additional work is required to ensure that the results are as accurate as possible. For example, it was expected that the shear layer, and thus the flame, would flap more than has been predicted here. A Fast Fourier Transform applied to preliminary calculations with a time step of one microsecond) showed that the dominant frequency in the flow was approximately 800 Hz with a secondary frequency of approximately 1200 Hz. Thus, it was determined that a time step of 5 microseconds would be sufficient to resolve the higher frequency. However, another Fast Fourier Transform performed after the calculation was complete showed that the dominant frequency fell to 500 Hz and the secondary rose to 2000 Hz. While steps of 5 microseconds are still sufficient to resolve these frequencies, the change in frequencies suggests that there may be some temporal diffusion affecting the solution.

Another example of where additional work on this problem should be performed is with the grid. The grid should be further refined in the vicinity of the shear layer to determine if any relevant physics are being missed and whether there is an over-prediction of gas diffusion, for instance. Too much diffusion could lead to erroneous results when predicting flame thickness or heat release.

It is important to undergo this process of learning how to properly set up, execute, and analyze three-dimensional simulations for this class of problems. Even though the current single-element problem is relatively simple—at least in comparison to more realistic rocket engines—these issues will become more important when trying to predict the acoustic map of the chamber or in understanding combustion instability. Small errors such as spatial or temporal diffusion, or grid resolution could greatly impact the predictions that are very sensitive to those errors. Learning how best to perform these types of calculations will go a long way towards trying to understand more complex rocket engine phenomena.

Summary and Conclusions

Three-dimensional calculations were performed on a single-element, shear-coaxial, gas/gas, H_2/O_2 rocket in an ongoing effort to develop a computational methodology to be used to predict rocket engine flow fields. The results from these calculations were compared to previous two-dimensional solutions to help determine the level of model fidelity that is required to reproduce the essential physical behavior of the flow. Such a determination will help make future calculations more efficient and robust.

The results showed a marked difference between the steady and time-averaged solutions. The steady solution is not able to capture the flapping of the flame, thus resulting in a thinner predicted flame. It was also shown that the three-dimensional calculations appeared to better represent the experimental data in the cases of the hydrogen and velocity profiles at five-inches from the injectors. However, because no uncertainties for the experimental data are currently available, it is difficult to make a definitive conclusion as to which level of fidelity is the most appropriate. The oxygen profiles from the various levels of fidelity are quantitatively similar near the centerline and into the shear layer, but the three-dimensional time-accurate calculation tends to deviate from the data on the outer edge of the shear layer. The RMS velocity profiles for all the degrees of fidelity are very similar, suggesting that the level of fidelity is not as important in trying to predict the turbulence levels as would be the turbulence model.

It was also shown that the pattern of concentration of nitrogen used to cool the optical access changes when comparing a two-dimensional axisymmetric calculation and a three-dimensional calculation. The three-dimensional calculation showed that the upstream recirculation zone is slightly forward from the one predicted by the two-dimensional simulation. This caused some of the nitrogen to be pulled into the recirculation zone and moved upstream where it collected in small quantities in the corners of the modeled chamber. This is important for researchers using CFD to design an experiment.

Finally, there was no evidence that any three-dimensional flow patterns exist in the shear layer. It had originally been thought that some type of helical structure may be present, but streamtrace analyses and time-histories of transverse slices through the volume data showed no such structures. This suggests that fully three-dimensional models may not be necessary and that one can still obtain reasonable accuracy from planar or wedge symmetric models, thus increasing the efficiency of such calculations.

These results come from the highest fidelity simulations run on this problem to date. Yet, continued study is needed to further advance the performance of these three-dimensional, time-accurate calculations. The effects of grid and temporal refinement should be investigated to ensure that essential physics of the flow are not being overlooked. It seems that the CFD community is only at the edge of learning how to perform these types of simulations for this class of problems, and it will be necessary to fully understand the subtleties of these problems and their setup when one is ready to investigate phenomena such as acoustics or combustion instability.

References

1. Moser, M. D., Merenich, J. J., Pal, S., & Santoro, R. J., "OH-Radical Imaging and Velocity Field Measurements in a Gaseous Hydrogen/Oxygen Rocket," AIAA 93-2036, 29th AIAA/SAE/ASME/ASEE Joint Propulsion Conference & Exhibit, Monterey, CA, June 1993.

2. Foust, M. J., Deshpande, M., Pal, S., Ni, T., Merkle, C. L., & Santoro, R. J., "Experimental and Analytical Characterization of a Shear Coaxial Combusting GO_2/GH_2 Flowfield," AIAA 96-0646, AIAA 34th Aerospace Sciences Meeting & Exhibit, Reno, NV, Jan. 1996.

3. Schley, C. –A., Gagemann, G., & Golovitchev, V., "Comparison of High Pressure H_2/O_2 Rocket Model Engine Reference Simulations," AIAA 95-2429, 31st AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, San Diego, CA, July 1995.

4. Schley, C. –A., Gagemann, G., Tucker, P. K., Venkateswaran, S., & Merkle, C. L., "Comparison of Computational Codes for Modeling Hydrogen-Oxygen Injectors," AIAA 97-3302, 33rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, Seattle, WA, July 1997.

5. Archambault, M. R., Talley, D., & Peroomian, O., "Computational Analysis of a Single-Element Shear-Coaxial, GH_2/GO_2 Engine," AIAA 2002-1088, 40th Aerospace Sciences Meeting & Exhibit, Reno, NV, Jan. 2002.

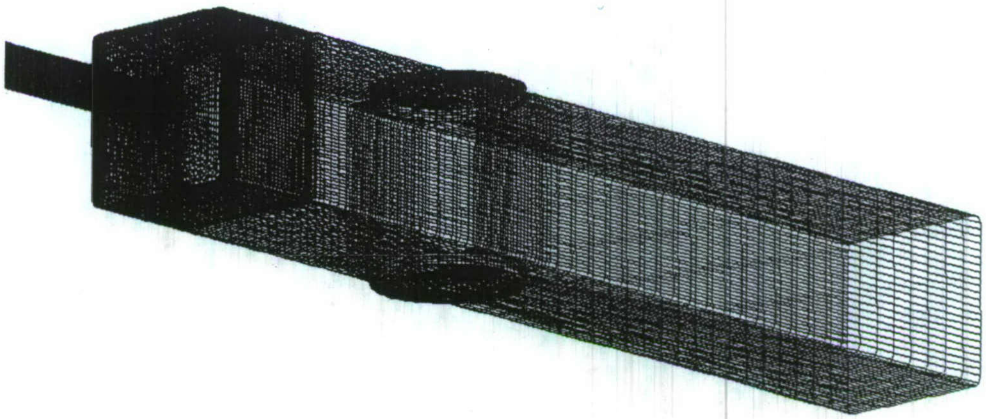
6. Archambault, M. R. & Peroomian, O., "Characterization of a Gas/Gas, Hydrogen/Oxygen Engine," AIAA 2002-3594, 38th AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, Indianapolis, IN, July 2002.

7. Chakravarthy, S., & Peroomian, O., "Some Internal Flow Applications of a Unified-Grid CFD Methodology," AIAA 96-2926, 32nd AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, Lake Buena Vista, FL, July 1996.

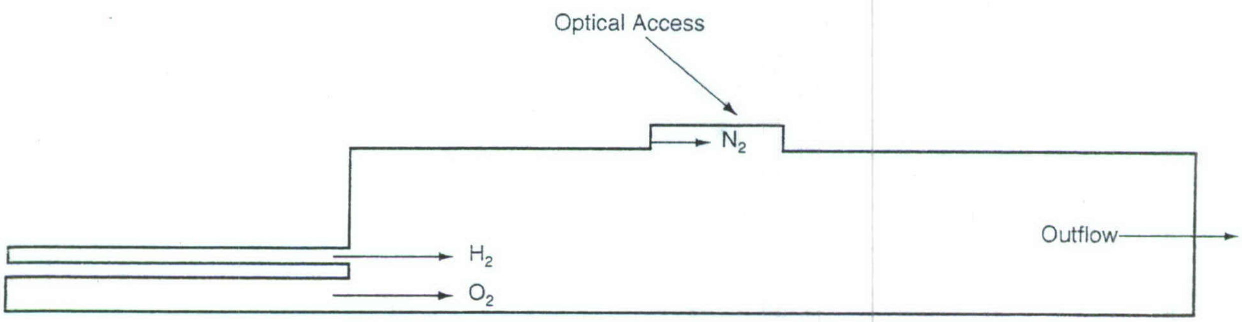
8. Peroomian, O., Chakravarthy, S., & Goldberg, U., "A 'Grid-Transparent' Methodology for CFD," AIAA 97-0724, 35th Aerospace Sciences Meeting & Exhibit, Reno, NV, Jan. 1997.

9. Anderson, J. D., *Hypersonic and High Temperature Gas Dynamics*, McGraw-Hill, 1989, Table 13.2.

10. Goldberg, U., Peroomian, O., & Chakravarthy, S., "A Wall-Distance-Free k-e Model With Enhanced Near-Wall Treatment," ASME J. Fluids Eng. 120, 1998, 457-462.

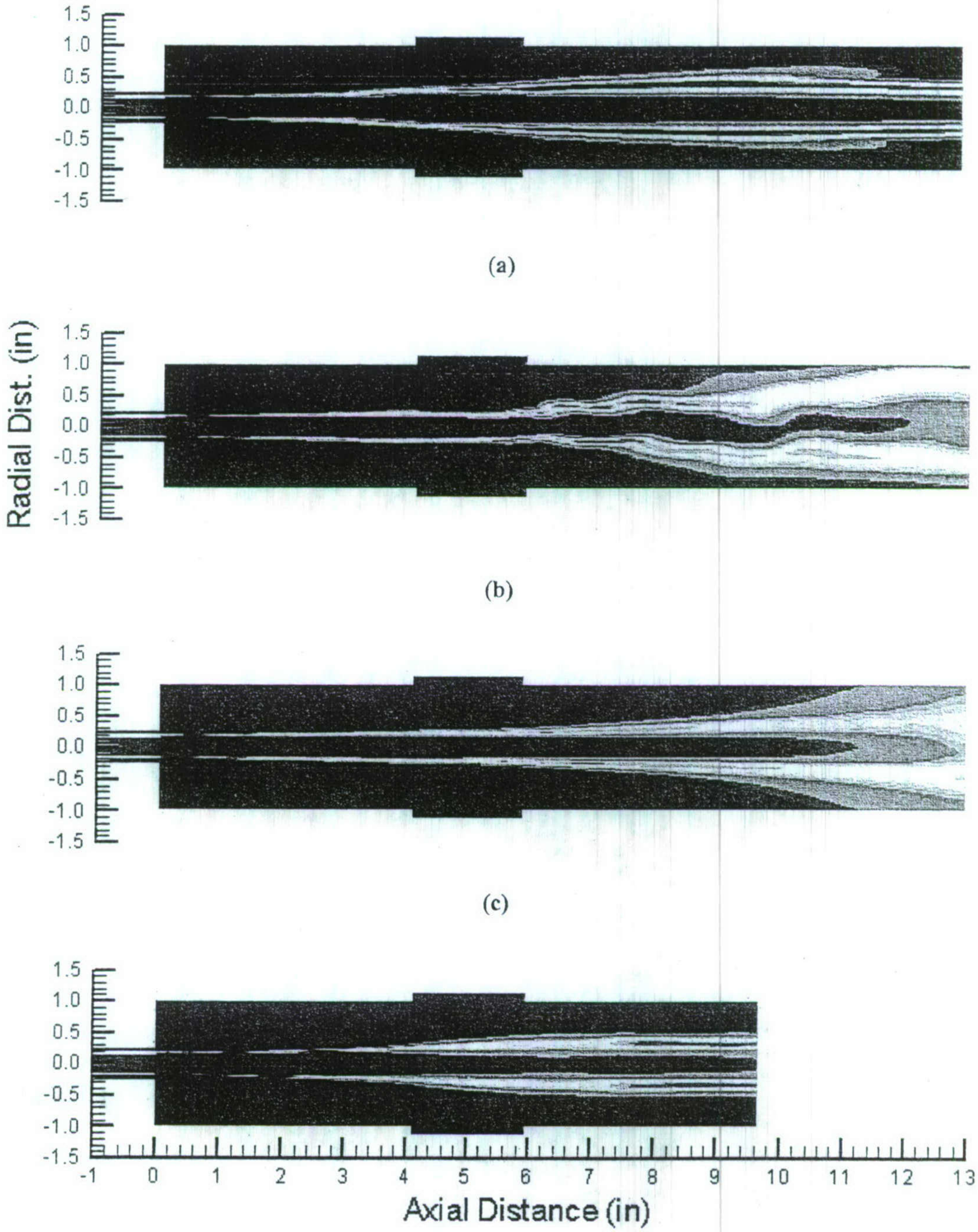


(a)



(b)

Figure 1. Schematic of computational domain.



(a)

(b)

(c)

(d)

Figure 2. OH concentration contours from (a) 3-D steady, (b) 3-D instantaneous, (c) 3-D time-averaged, and (d) 2-D time averaged solutions.

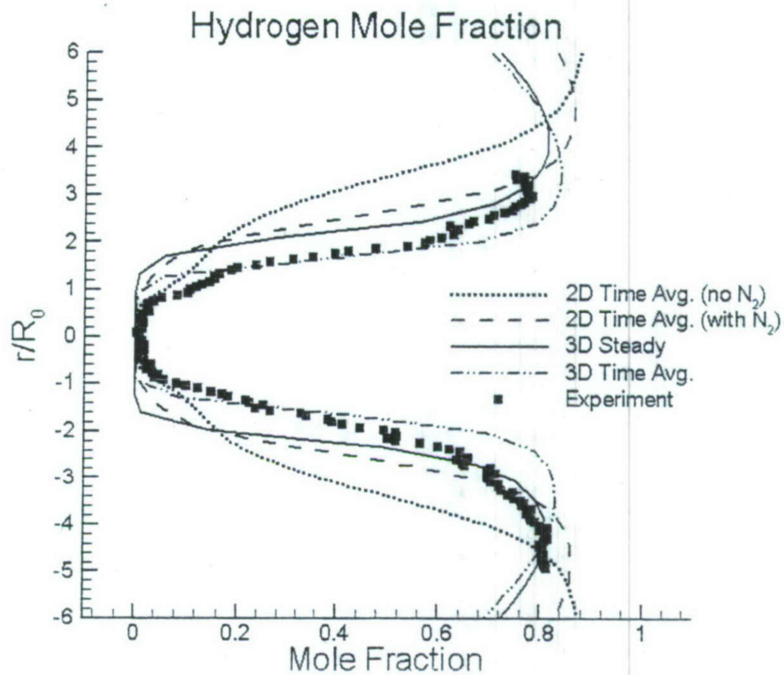


Figure 3. Hydrogen mole fraction profiles five inches downstream from injector.

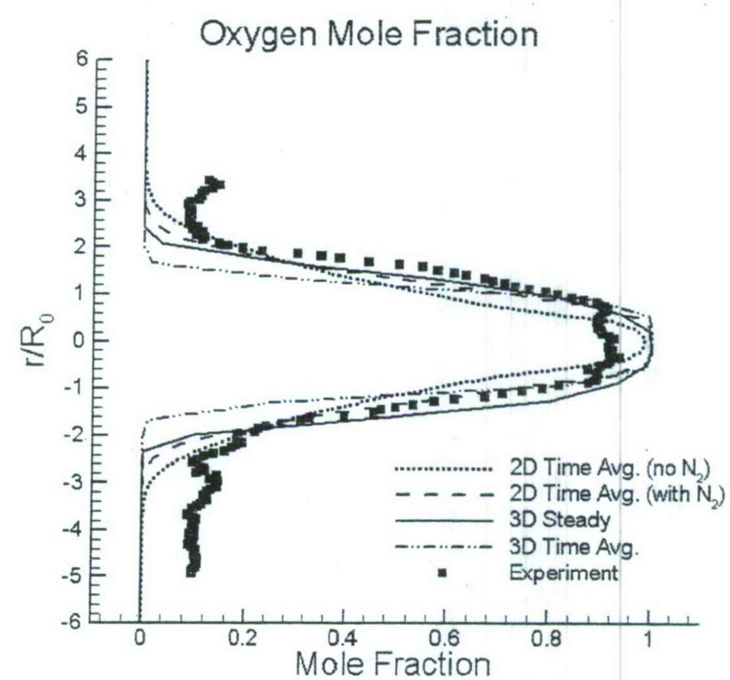


Figure 4. Oxygen mole fraction profiles five inches downstream from injector.

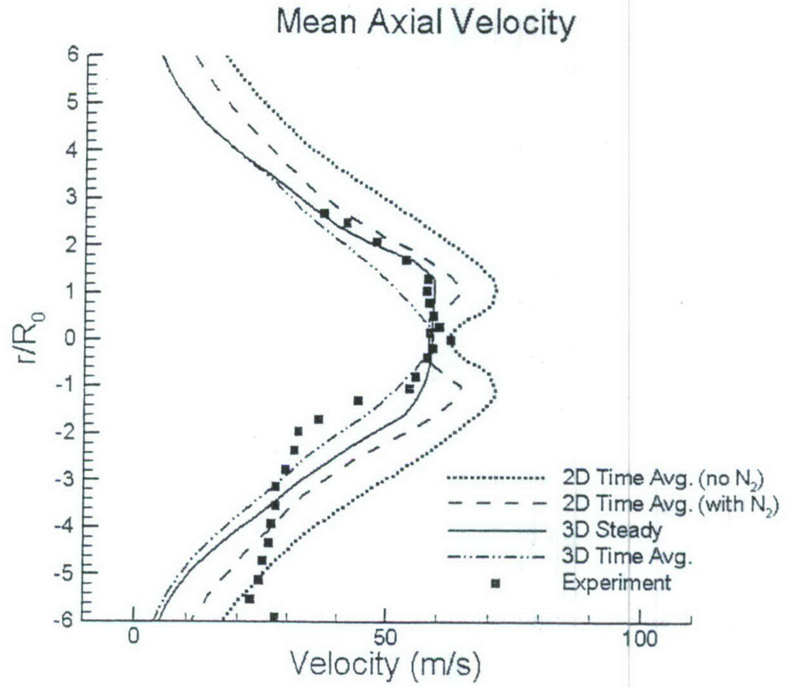


Figure 5. Mean axial velocity profiles at five inches downstream from injector.

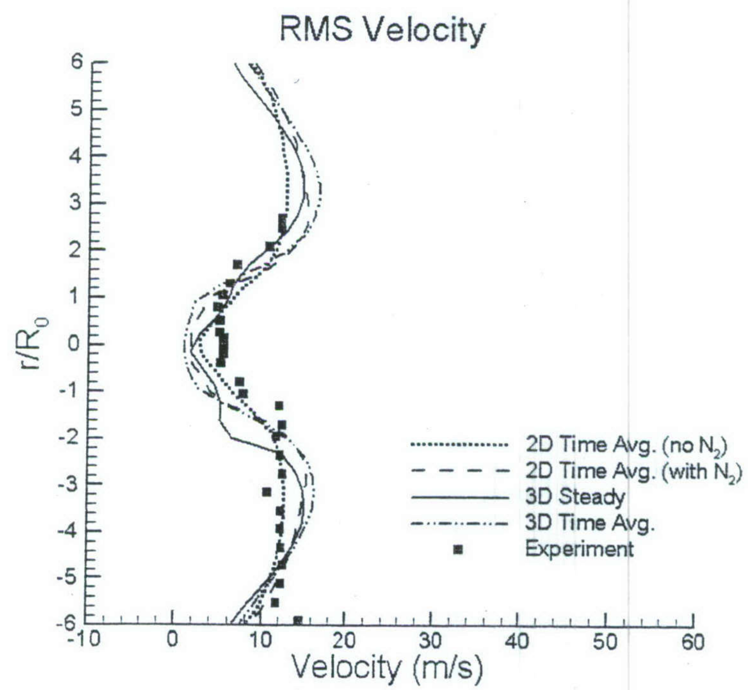


Figure 6. RMS velocity profiles at five inches downstream from injector.

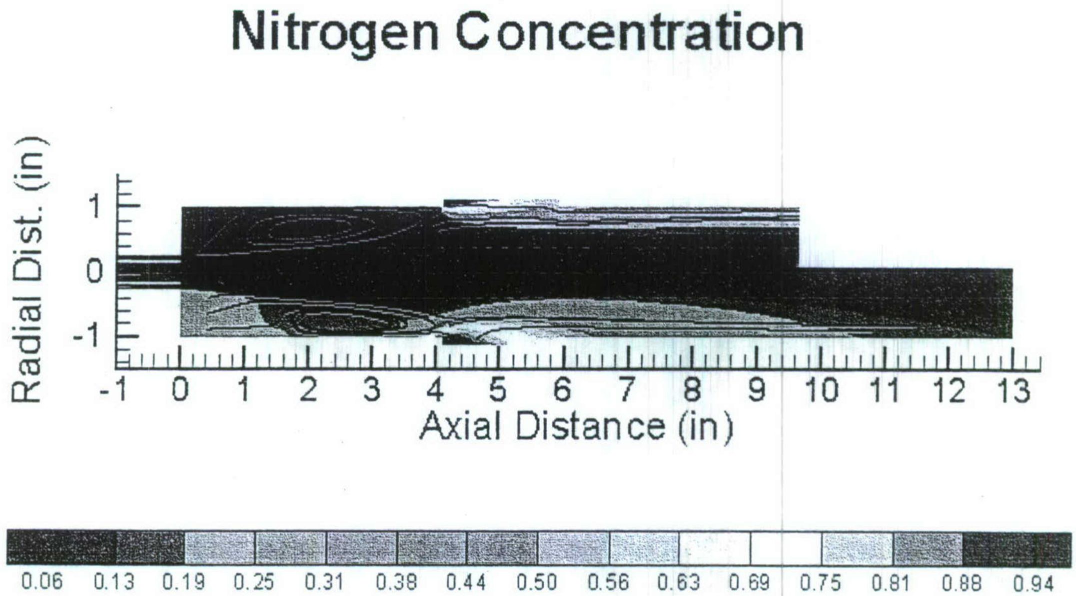


Figure 7. Comparison of 2-D axisymmetric (top half) and 3-D time-averaged nitrogen contours and streamtraces.

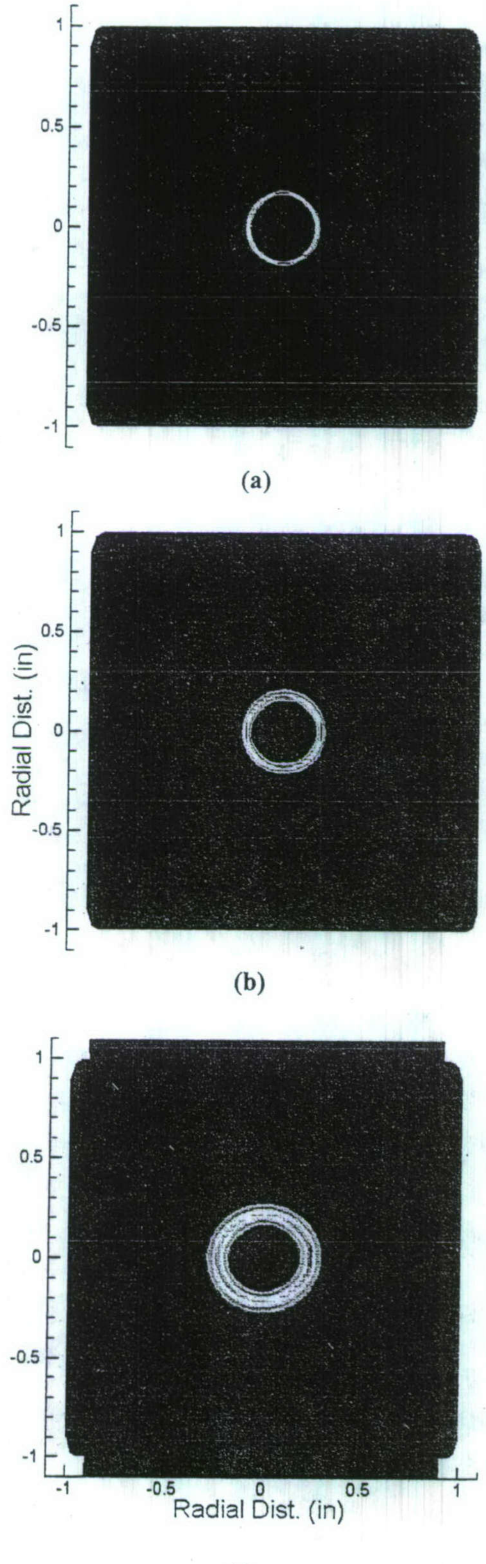


Figure 8. OH contours from transverse planes located at (a) 1 in, (b) 2 in, and (c) 5 in downstream from injector.